



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:03 AM GMT

PDB ID : 1E8V  
Title : STRUCTURE OF THE MULTIFUNCTIONAL PARAMYXOVIRUS HEMA  
GGLUTININ-NEURAMINIDASE  
Authors : Crennell, S.; Takimoto, T.; Portner, A.; Taylor, G.  
Deposited on : 2000-10-01  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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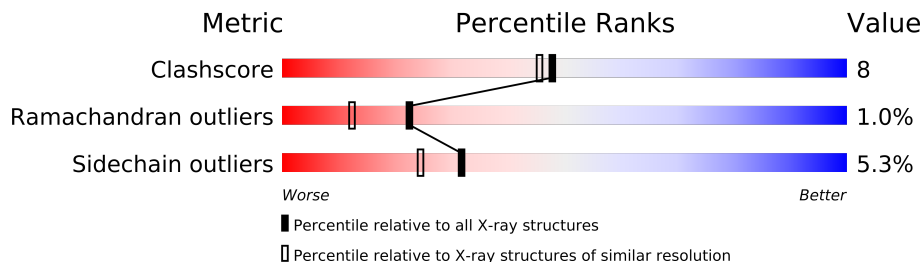
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7245 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

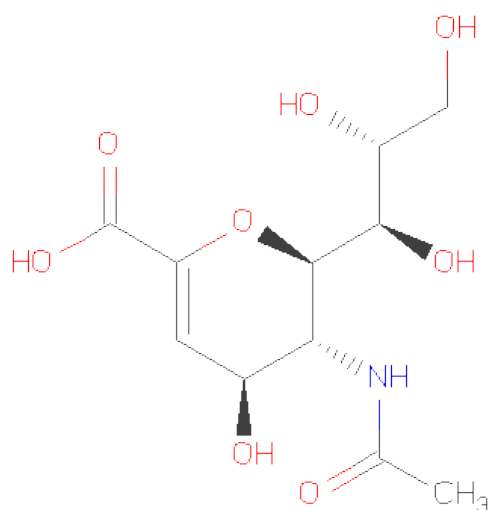
- Molecule 1 is a protein called HEMAGGLUTININ-NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3449	2174	588	668	19			
1	B	446	Total	C	N	O	S	0	0	0
			3445	2172	587	667	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

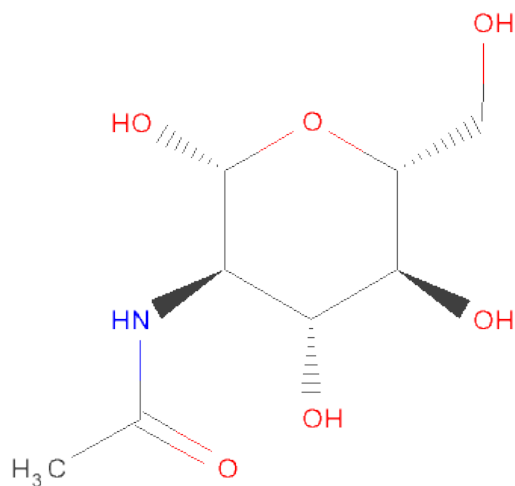
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINICACID (three-letter code: DAN) (formula: C<sub>11</sub>H<sub>17</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	11	1	8		
3	B	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	110	Total 110	O 110	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

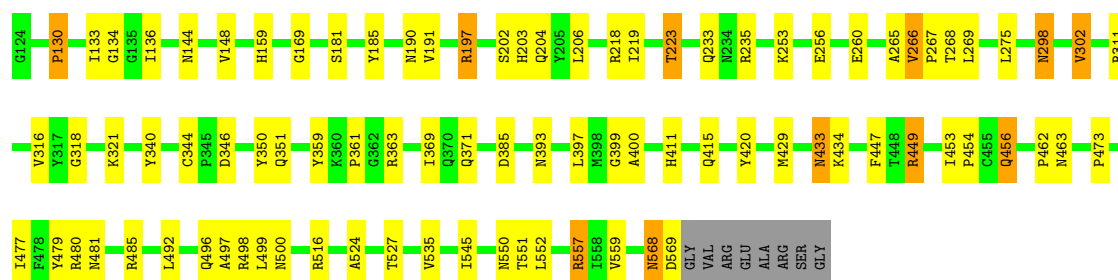
#### • Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

Chain A: 



#### • Molecule 1: HEMAGGLUTININ-NEURAMINIDASE

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.46Å 137.46Å 116.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.0 (6.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, DAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/3534	0.77	3/4807 (0.1%)
1	B	0.39	0/3530	0.74	3/4802 (0.1%)
All	All	0.39	0/7064	0.75	6/9609 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	1	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	449	ARG	NE-CZ-NH2	-17.13	111.73	120.30
1	A	449	ARG	NE-CZ-NH1	15.55	128.08	120.30
1	B	449	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	B	449	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	449	ARG	CD-NE-CZ	8.08	134.91	123.60
1	B	449	ARG	CD-NE-CZ	6.32	132.45	123.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1571	NAG	C1

There are no planarity outliers.



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3449	0	3342	53	0
1	B	3445	0	3339	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	16	0	0
3	B	20	0	16	0	0
4	A	28	0	26	2	0
4	B	14	0	13	0	0
5	B	28	0	25	1	0
6	A	129	0	0	5	0
6	B	110	0	0	4	0
All	All	7245	0	6777	109	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:THR:HG21	6:A:2032:HOH:O	1.69	0.91
1:B:223:THR:HG21	6:B:2034:HOH:O	1.89	0.72
1:A:197:ARG:H	1:A:197:ARG:HD3	1.61	0.66
1:B:197:ARG:H	1:B:197:ARG:HD3	1.63	0.64
1:A:453:ILE:HG13	1:A:496:GLN:NE2	2.12	0.63
1:B:453:ILE:HG13	1:B:496:GLN:NE2	2.14	0.61
6:A:2047:HOH:O	1:B:223:THR:HG23	1.99	0.61
1:B:185:TYR:OH	1:B:223:THR:HG22	2.01	0.60
1:B:568:ASN:O	1:B:569:ASP:HB2	2.02	0.60
1:B:371:GLN:HE22	1:B:400:ALA:H	1.48	0.59
1:B:481:ASN:CG	5:B:1571:NAG:HN2	2.06	0.59
1:A:453:ILE:HA	1:A:456:GLN:NE2	2.18	0.58
1:A:371:GLN:HE22	1:A:400:ALA:H	1.49	0.58
1:B:190:ASN:HD22	1:B:204:GLN:NE2	2.00	0.58
1:A:550:ASN:HB2	1:A:557:ARG:HG2	1.86	0.58
1:A:185:TYR:OH	1:A:223:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ASN:HD22	1:A:204:GLN:NE2	2.02	0.57
4:A:1573:NAG:C3	4:A:1573:NAG:O7	2.52	0.57
1:B:453:ILE:HA	1:B:456:GLN:NE2	2.19	0.56
1:A:233:GLN:NE2	1:A:253:LYS:HD3	2.20	0.56
1:A:371:GLN:NE2	1:A:400:ALA:H	2.04	0.55
1:B:479:TYR:CD1	1:B:485:ARG:HD2	2.41	0.55
1:A:266:VAL:HG12	1:A:267:PRO:HD2	1.90	0.54
1:B:371:GLN:NE2	1:B:400:ALA:H	2.04	0.54
1:A:344:CYS:SG	1:A:351:GLN:NE2	2.81	0.54
1:B:134:GLY:HA2	6:B:2003:HOH:O	2.08	0.54
1:A:223:THR:HG23	6:B:2044:HOH:O	2.07	0.53
1:A:479:TYR:CD1	1:A:485:ARG:HD2	2.43	0.53
1:A:454:PRO:HA	1:A:456:GLN:HE22	1.72	0.53
1:B:266:VAL:HG12	1:B:267:PRO:HD2	1.89	0.53
1:B:169:GLY:HA2	1:B:552:LEU:O	2.08	0.53
1:B:233:GLN:NE2	1:B:253:LYS:HD3	2.24	0.53
1:B:454:PRO:HA	1:B:456:GLN:HE22	1.73	0.53
1:A:169:GLY:HA2	1:A:552:LEU:O	2.09	0.53
1:B:371:GLN:HE21	1:B:399:GLY:HA2	1.75	0.52
1:B:550:ASN:HB2	1:B:557:ARG:HG2	1.91	0.52
1:A:191:VAL:O	1:A:202:SER:HB2	2.11	0.51
1:B:361:PRO:HD2	1:B:369:ILE:HD13	1.93	0.50
1:B:344:CYS:SG	1:B:351:GLN:NE2	2.84	0.50
1:B:191:VAL:O	1:B:202:SER:HB2	2.11	0.50
1:B:369:ILE:HD12	1:B:369:ILE:N	2.27	0.49
1:A:361:PRO:HD2	1:A:369:ILE:HD13	1.95	0.49
1:B:420:TYR:CG	1:B:462:PRO:HA	2.48	0.49
1:B:498:ARG:HB3	1:B:524:ALA:O	2.13	0.49
1:A:371:GLN:HE21	1:A:399:GLY:HA2	1.78	0.48
1:B:527:THR:HA	1:B:545:ILE:O	2.13	0.48
1:A:420:TYR:CG	1:A:462:PRO:HA	2.48	0.48
1:A:144:ASN:OD1	1:A:480:ARG:HG3	2.13	0.48
1:A:369:ILE:N	1:A:369:ILE:HD12	2.29	0.48
1:A:411:HIS:HB2	1:A:429:MET:O	2.14	0.47
1:B:268:THR:H	1:B:298:ASN:HD21	1.62	0.47
1:B:479:TYR:CE2	1:B:485:ARG:HG2	2.49	0.47
1:B:136:ILE:HG21	1:B:181:SER:O	2.15	0.47
1:A:206:LEU:HD13	1:A:275:LEU:HB2	1.96	0.47
1:A:268:THR:H	1:A:298:ASN:HD21	1.62	0.46
1:B:144:ASN:OD1	1:B:480:ARG:HG3	2.15	0.46
1:B:148:VAL:HG13	1:B:477:ILE:HD12	1.98	0.46
1:A:479:TYR:CE2	1:A:485:ARG:HG2	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:533:LYS:HE2	6:A:2115:HOH:O	2.15	0.46
1:A:527:THR:HA	1:A:545:ILE:O	2.15	0.46
1:B:456:GLN:H	1:B:456:GLN:NE2	2.14	0.46
1:A:318:GLY:O	1:A:369:ILE:HA	2.16	0.46
1:B:497:ALA:HB3	1:B:499:LEU:HD12	1.97	0.46
1:B:206:LEU:HD13	1:B:275:LEU:HB2	1.97	0.45
1:A:498:ARG:HB3	1:A:524:ALA:O	2.16	0.45
1:B:318:GLY:O	1:B:369:ILE:HA	2.16	0.45
1:A:501:PRO:HD2	6:A:2106:HOH:O	2.16	0.45
1:A:456:GLN:NE2	1:A:456:GLN:H	2.15	0.45
1:A:497:ALA:HB3	1:A:499:LEU:HD12	1.97	0.45
1:B:551:THR:O	1:B:552:LEU:HB2	2.16	0.45
1:B:371:GLN:NE2	1:B:415:GLN:HE21	2.15	0.44
6:A:2009:HOH:O	1:B:203:HIS:HE1	2.01	0.44
1:A:516:ARG:HH11	1:A:516:ARG:HG2	1.82	0.44
1:B:218:ARG:NH2	6:B:2041:HOH:O	2.51	0.43
1:A:256:GLU:HG2	1:A:256:GLU:H	1.69	0.43
1:B:433:ASN:HB3	1:B:434:LYS:H	1.46	0.43
1:A:371:GLN:NE2	1:A:415:GLN:HE21	2.15	0.43
1:A:202:SER:OG	1:A:236:LYS:HE3	2.18	0.43
1:B:516:ARG:HG2	1:B:516:ARG:HH11	1.83	0.43
1:A:197:ARG:CD	1:A:197:ARG:H	2.23	0.43
1:B:256:GLU:HB2	1:B:260:GLU:HB2	2.01	0.43
1:A:136:ILE:HG21	1:A:181:SER:O	2.20	0.42
1:A:268:THR:H	1:A:298:ASN:ND2	2.18	0.42
1:A:148:VAL:HG13	1:A:477:ILE:HD12	2.02	0.42
1:A:433:ASN:HB3	1:A:434:LYS:H	1.46	0.42
1:A:346:ASP:HB3	1:A:350:TYR:HD2	1.85	0.42
1:B:411:HIS:HB2	1:B:429:MET:O	2.20	0.42
1:B:130:PRO:HA	1:B:133:ILE:HG12	2.01	0.42
1:B:311:ARG:NH2	1:B:385:ASP:O	2.52	0.42
1:B:190:ASN:HD22	1:B:204:GLN:HE21	1.67	0.42
1:A:551:THR:O	1:A:552:LEU:HB2	2.20	0.41
1:A:311:ARG:NH2	1:A:385:ASP:O	2.52	0.41
1:B:268:THR:H	1:B:298:ASN:ND2	2.19	0.41
1:A:130:PRO:HA	1:A:133:ILE:HG12	2.01	0.41
1:A:185:TYR:HH	1:A:223:THR:HG22	1.86	0.41
1:B:256:GLU:HG2	1:B:256:GLU:H	1.72	0.41
1:B:235:ARG:HG3	1:B:235:ARG:HH11	1.86	0.41
4:A:1573:NAG:O7	4:A:1573:NAG:H3	2.20	0.41
1:B:420:TYR:CD1	1:B:462:PRO:HA	2.56	0.41
1:A:256:GLU:HB2	1:A:260:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:ALA:O	1:A:321:LYS:HE2	2.21	0.41
1:B:359:TYR:CE2	1:B:393:ASN:HB3	2.56	0.41
1:A:359:TYR:CE2	1:A:393:ASN:HB3	2.56	0.41
1:B:453:ILE:HA	1:B:456:GLN:HE21	1.85	0.40
1:B:265:ALA:O	1:B:321:LYS:HE2	2.21	0.40
1:A:190:ASN:HD22	1:A:204:GLN:HE21	1.66	0.40
1:B:346:ASP:HB3	1:B:350:TYR:HD2	1.85	0.40
1:A:470:TYR:O	1:A:526:TYR:HA	2.22	0.40
1:A:481:ASN:O	1:A:482:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/454 (98%)	410 (92%)	31 (7%)	4 (1%)	25	14
1	B	444/454 (98%)	408 (92%)	31 (7%)	5 (1%)	21	10
All	All	889/908 (98%)	818 (92%)	62 (7%)	9 (1%)	22	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ARG
1	B	363	ARG
1	B	568	ASN
1	A	302	VAL
1	A	473	PRO
1	B	473	PRO
1	B	302	VAL
1	A	500	ASN
1	B	500	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/392 (99%)	367 (95%)	20 (5%)	32	25
1	B	387/392 (99%)	366 (95%)	21 (5%)	31	24
All	All	774/784 (99%)	733 (95%)	41 (5%)	32	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	197	ARG
1	A	219	ILE
1	A	223	THR
1	A	266	VAL
1	A	269	LEU
1	A	298	ASN
1	A	316	VAL
1	A	340	TYR
1	A	397	LEU
1	A	431	VAL
1	A	433	ASN
1	A	447	PHE
1	A	449	ARG
1	A	456	GLN
1	A	463	ASN
1	A	492	LEU
1	A	535	VAL
1	A	557	ARG
1	A	559	VAL
1	B	130	PRO
1	B	159	HIS
1	B	197	ARG
1	B	219	ILE
1	B	223	THR
1	B	266	VAL
1	B	269	LEU
1	B	298	ASN
1	B	302	VAL

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Mol	Chain	Res	Type
1	B	316	VAL
1	B	340	TYR
1	B	397	LEU
1	B	433	ASN
1	B	447	PHE
1	B	449	ARG
1	B	456	GLN
1	B	463	ASN
1	B	492	LEU
1	B	535	VAL
1	B	557	ARG
1	B	559	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	298	ASN
1	A	351	GLN
1	A	371	GLN
1	A	456	GLN
1	A	463	ASN
1	A	496	GLN
1	B	204	GLN
1	B	298	ASN
1	B	351	GLN
1	B	371	GLN
1	B	456	GLN
1	B	463	ASN
1	B	496	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1571	1,5	12,14,15	1.60	2 (16%)	15,19,21	1.06	1 (6%)
5	NAG	B	1572	5	12,14,15	0.67	0	15,19,21	0.96	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1571	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	1572	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1571	NAG	C4-C5	-3.83	1.44	1.53
5	B	1571	NAG	C4-C3	-2.66	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1572	NAG	C3-C2-N2	-2.93	107.30	111.76
5	B	1571	NAG	C3-C2-N2	-2.90	107.34	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1571	NAG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DAN	A	1571	-	20,20,20	2.28	6 (30%)	28,28,28	2.01	6 (21%)
4	NAG	A	1572	1	12,14,15	1.34	1 (8%)	15,19,21	1.03	1 (6%)
4	NAG	A	1573	1	12,14,15	1.09	1 (8%)	15,19,21	0.88	1 (6%)
3	DAN	B	1570	-	20,20,20	1.78	4 (20%)	28,28,28	2.14	7 (25%)
4	NAG	B	841	1	12,14,15	1.51	2 (16%)	15,19,21	1.44	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAN	A	1571	-	-	0/18/34/34	0/1/1/1
4	NAG	A	1572	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1573	1	-	1/6/23/26	0/1/1/1
3	DAN	B	1570	-	-	0/18/34/34	0/1/1/1
4	NAG	B	841	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1571	DAN	C6-C5	5.54	1.62	1.53
3	A	1571	DAN	C3-C2	4.80	1.42	1.33
4	B	841	NAG	C3-C2	4.47	1.61	1.52
3	A	1571	DAN	C4-C3	4.38	1.56	1.50
3	B	1570	DAN	C3-C2	4.36	1.41	1.33
3	B	1570	DAN	C4-C3	4.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1572	NAG	C3-C2	3.90	1.60	1.52
3	A	1571	DAN	C2-C1	-2.84	1.41	1.48
3	B	1570	DAN	C2-C1	-2.73	1.41	1.48
3	A	1571	DAN	C5-N5	2.56	1.50	1.45
3	A	1571	DAN	C4-C5	2.41	1.56	1.52
4	B	841	NAG	C2-N2	2.15	1.48	1.46
4	A	1573	NAG	O5-C5	-2.10	1.41	1.45
3	B	1570	DAN	C7-C6	-2.05	1.50	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1570	DAN	O6-C2-C1	6.34	124.39	111.88
3	A	1571	DAN	C6-O6-C2	6.33	124.19	114.72
3	B	1570	DAN	O6-C2-C3	-4.91	117.97	124.33
4	B	841	NAG	C3-C2-N2	-4.76	104.52	111.76
3	B	1570	DAN	C6-O6-C2	4.31	121.16	114.72
3	A	1571	DAN	O6-C2-C1	3.83	119.43	111.88
3	A	1571	DAN	C3-C2-C1	-3.38	117.46	124.12
3	B	1570	DAN	C3-C2-C1	-3.30	117.63	124.12
3	A	1571	DAN	O4-C4-C3	3.19	117.25	109.67
3	A	1571	DAN	C7-C6-C5	-3.08	109.70	114.24
4	A	1572	NAG	C3-C2-N2	-2.54	107.89	111.76
4	A	1573	NAG	C3-C2-N2	2.52	115.59	111.76
3	B	1570	DAN	C4-C5-N5	-2.43	106.59	111.04
3	B	1570	DAN	C7-C6-C5	-2.33	110.81	114.24
3	B	1570	DAN	C8-C7-C6	-2.06	109.00	112.99
3	A	1571	DAN	O6-C2-C3	-2.03	121.70	124.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1572	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1573	NAG	C3-C2-N2-C7

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.